Bayesian Estimation of the Transmissivity Spatial Structure from Pumping Test Data

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ABSTRACT

Estimating the statistical parameters (mean, variance, and integral scale) that define the spatial structure of the transmissivity or hydraulic conductivity fields is a fundamental step for the accurate prediction of subsurface flow and contaminant transport. In practice, the determination of the spatial structure is a challenge because of spatial heterogeneity and data scarcity. In this paper, we describe a novel approach that uses time drawdown data from multiple pumping tests to determine the transmissivity statistical spatial structure. The method builds on the pumping test interpretation procedure of Copty et al. (2011) (Continuous Derivation method, CD), which uses the time-drawdown data and its time derivative to estimate apparent transmissivity values as a function of radial distance from the pumping well. A Bayesian approach is then used to infer the statistical parameters of the transmissivity field by combining prior information about the parameters and the likelihood function expressed in terms of radially-dependent apparent transmissivities determined from pumping tests. A major advantage of the proposed Bayesian approach is that the likelihood function is readily determined from randomly generated multiple realizations of the transmissivity field, without the need to solve the groundwater flow equation. Applying the method to synthetically-generated pumping test data, we demonstrate that, through a relatively simple procedure, information on the spatial structure of the transmissivity may be inferred from pumping tests data. It is also shown that the prior parameter distribution has a significant influence on the estimation procedure, given the non-uniqueness of the estimation procedure. Results also indicate that the reliability of the estimated transmissivity statistical parameters increases with the number of available pumping tests.

1. INTRODUCTION

The modeling of groundwater flow and contaminant transport has evolved in recent decades into a valuable tool for the analysis of subsurface systems. Such modeling efforts require mapping the flow parameters - most notably transmissivity (T) or hydraulic conductivity (K) - over the domain of interest. Numerous field investigations have however demonstrated that hydrogeological parameters are highly heterogeneous, displaying complex patterns of spatial variability (e.g., *Gelhar* 1993; *Rubin*, 2003, Sudicky et al. 2010). Because flow and transport are strongly influenced by the heterogeneity of the subsurface system, incorporating the spatial variability of the underlying parameters is essential for the accurate evaluation of groundwater resources, and in particular for the prediction of contaminant transport as a necessary step for the design and implementation of groundwater remediation activities (e.g., *Sanchez-Vila and Fernandez-Garcia,* 2016).

Complexity in hydrogeological patterns and the lack of detailed data have led researchers to formulate the flow and transport problem within a stochastic framework. With such an approach, flow parameters are defined by spatial random functions whose spatial structure can adequately be expressed in terms of few low-order statistical parameters, namely the spatial mean, variance, and integral scale, which jointly define the covariance function or semi-variogram (*Kitanidis*, 1997; *Renard*, 2007). These statistical parameters are typically determined from measurements of the attribute of interest, provided that a sufficiently large number of data with adequate spatial coverage is available.

Groundwater flow and solute transport are strongly affected by the spatial distribution of T. At most sites, the number of T estimates determined from the interpretation of pumping tests is quite limited, hindering the accurate determination of the T covariance function. Moreover, traditional pumping test interpretation methods, such as those based on log-log plots (*Theis*, 1935) or semilog plots (*Cooper and Jacob*, 1946), generally yield single estimates of the flow parameters, which hardly provide information about the underlying heterogeneity. In fact, this averaging process results in T estimates with a smaller variance and a larger integral scale as compared to the actual point distributions, and hence, cannot be used to simulate the impact of small to medium scale variability, which is of interest in many field applications.

These limitations motivated many researchers in the last three decades to examine the impact of spatial heterogeneity on the analysis of pumping tests and investigate whether information about the spatial variability of the flow parameters can be inferred from pumping tests (a

review of methods and solutions was provided by *Sanchez-Vila et al.*, 2006). A very early study is *Barker and Herbert* (1982), who considered the effect of a high hydraulic conductivity anomaly embedded in an otherwise uniform aquifer. *Butler* (1988) used the *Cooper and Jacob* (1946) method to investigate the effect of a *T* anomaly on the interpreted transmissivity; it was shown that, for observation wells located at large distances from the pumping well, the perturbed non-uniform aquifer behaves as a homogeneous aquifer. On the other hand, *Butler* (1990) showed that the *T* values estimated with the *Theis* (1935) method place more weight on the local *T*, defined as the *T* in the vicinity of the pumping well. Feitosa et al. (1994) developed an inverse procedure for the estimation of the transmissivity as a function of distance from the pumping well for the case when the transmissivity field consists of a series of concentric homogeneous rings.

For spatially variable *T* fields (i.e., *T* fields that are not defined in terms of a deterministic perturbation but that are individual realizations of a random field), *Meier et al.* (1998) and *Sanchez-Vila et al.* (1999) showed that the transmissivity obtained with the *Cooper and Jacob* (1946) is close to the spatial geometric mean of the *T* field, regardless of the location of the observation point. On the other hand, the estimated storativity (*S*) varies spatially, demonstrating how the interpretation method significantly translates the heterogeneity in transmissivity into spatially variable *S* estimates. This finding was further confirmed by *Trinchero et al.* (2008b), who provided an analytical relationship between the estimated storativity and the porosity inferred from tracer test data (the latter parameter was considered as an indicator of transport connectivity).

Copty and Findikakis (2004a) examined the sensitivity of transient drawdown in pumping tests to the statistical parameters describing the spatial structure of *T*, and noted that the time derivative of the drawdown is particularly sensitive to the heterogeneity in *T*. *Oliver* (1993) and *Knight and Kluitenberg* (2005) used the Frechet kernel to evaluate the sensitivity of the drawdown to the spatial variability of *T* and *S*. *Leven and Dietrich* (2006) used sensitivity coefficients to assess the influence of the spatial variability of *T* and *S* on the interpretation of pumping tests, leading to time-dependent interpreted parameters. *Avci et al.* (2011, 2013) developed a numerical method for the estimation of the variability of the *T* and *S* as a function of pumping time; the method could be used as a diagnostic tool to identify some aquifer system characteristics. *Avci et al.* (2014) evaluated the performance of a number of analytical methods for the estimation of the variation of the transmissivity with radial distance. Recently, *Pechstein et al.* (2016) discussed the relationship of the interpreted *T*

values derived from pumping tests to the underlying spatial variability of the T field. The authors showed numerically that the interpreted T value that best reproduces the pumping test data in confined heterogeneous aquifers is a weighted average of the point T values which uses the temporal derivative of the Frechet kernel as a spatial weight.

Copty et al. (2008) and *Trinchero et al.* (2008a) considered the influence of spatial variability of the transmissivity on pumping tests conducted in leaky aquifers. A significant difference between flow towards a well in a confined non-leaky versus a leaky aquifer is that in the former case the cone of depression continues to expand with time, while in the latter a steady state condition is reached. As a result, the response of a pumping test in a leaky aquifer is more sensitive to variations in the local transmissivity in the vicinity of the well, as compared to the case of a confined aquifer.

A number of studies have attempted to estimate directly, from pumping test data, the statistical spatial structure of the transmissivity field, commonly expressed in terms of two statistical parameters: variance and integral scale. *Copty and Findikakis* (2004b) examined the relation of the time-derivative of the drawdown to the integral scale and the variance of the log-transmissivity field. *Neuman et al.* (2004, 2007) developed a graphical approach that uses steady-state drawdown data for the estimation of the T variance and integral scale. *Riva et al.* (2009) applied this type-curve method to field data from the site of Poitiers, France. *Firmani et al.* (2006) used an expression of the equivalent hydraulic conductivity for steady-state radially convergent flow towards a well in a heterogeneous aquifer to estimate the variance and integral scale of K. *Zech et al.* (2012) developed an analytical expression for the steady state drawdown due to pumping in a heterogeneous aquifer using the Coarse Graining upscaling method (*Attinger*, 2003), a method subsequently applied to real pumping test data from the Horkheimer Insel test site in Germany (*Zech et al.*, 2015). This latter paper also discusses the quantity and spatial coverage of the data needed to obtain reliable estimates of the statistical parameters of the transmissivity field. *Zech et al.* (2016) extended the analysis to transient flow and showed that the number of measurements needed to obtain reliable estimates of the transmissivity spatial structure is reduced compared to steady state pumping tests.

In parallel efforts, and to overcome the scarcity of hydrological data commonly encountered in field applications, a number of researchers have proposed incorporating additional secondary data in the identification of subsurface parameters such as geophysical data (see recent reviews such as *Binley et al.*, 2015; *Slater*, 2007; *Rubin and Hubbard*, 2005). Novel

field data acquisition techniques, such as hydraulic tomography (e.g., *Butler et al*., 1999; *Yeh, and Liu*, 2000; *Zhu and Yeh*, 2005; *Yin and Illman*, 2009; *Illman et al.*, 2015) and direct push technologies (*Butler et al.*, 2007; *Dietrich et al.*, 2008; *Bohling et al.,* 2012) have also been proposed. These approaches have been shown to have several benefits; most notably they allow for the collection of dense hydraulic head data in response to groundwater pumping that allows for the estimation of the three-dimensional hydraulic conductivity distribution in the vicinity of the tests. Despite these advantages, their application to routine field problems remains limited due to the relatively large costs associated and the difficulty of solving the groundwater inverse problem.

Despite these recent developments, the determination of the underlying statistical spatial structure of the transmissivity field from pumping test data remains a challenge. In a recent study, *Copty et al*. (2011) developed an interpretation method for pumping tests, denoted as the Continuous Derivation (CD) method. The CD method uses the transient drawdown data and its time derivative to estimate interpreted transmissivities as a function of the radial distance, $T_i(r)$. It was shown by *Copty et al.* (2011) that $T_i(r)$ is close to the geometric mean of the T values over a radially increasing volume, $T_g(r)$. The function $T_g(r)$ varies from the transmissivity at the well for small values of r, to the geometric mean of the entire field, for large r values. In the current study, we extend the work of *Copty et al.* (2011) by examining whether $T_i(r)$ can be used to infer the spatial structure of the transmissivity field. The goal is thus to develop a relatively simple pumping test interpretation method that can help in the definition of relevant characteristics of the local scale transmissivity spatial structure without the need for complex inverse modeling. We primarily focus on time-drawdown data derived from pumping tests, which remains a widely used technique for subsurface parameter estimation.

For the sake of completion, we present in Section 2 the main features of the CD method, followed by the presentation of the Bayesian approach used to infer the spatial structure of the transmissivity field, namely the variance and the integral scale. Section 3 describes a numerical application of the proposed Bayesian method and discusses its potential applications and limitations.

2. Pumping Test Interpretation Method

2.1. The Continuous Derivation Method (CD)

For pumping tests conducted in heterogeneous aquifers, the cone of depression due to pumping expands in time. At early times the apparent transmissivity is close to the T value in the immediate vicinity of the well (order of few meters), while at later times it is some weighted average of the transmissivity of a much larger region around the well. The term "apparent" is used here in accordance with the terminology of *Sanchez-Vila et al.*, 2006 which refers to an estimate of the parameter that is function of space and that satisfies some relationship such as the Theis solution (*Theis*, 1935). The CD method (*Copty et al.*, 2011) captures the full temporal transition between the local T value and the estimate obtained using late time data. The estimation method relies on the time-derivative of the drawdown because this is more sensitive than the drawdown itself to spatial variation of transmissivity (e.g., *Bourdet,* 2002).

For two-dimensional flow towards a well in a confined aquifer, the time-dependent drawdown is given by the classical Theis' solution: $s(t,r)=\frac{Q}{4\pi T}W(u)$, where $u=\frac{r^2 S}{4tT}$, $W(u)$ is the well (i.e., the exponential integral) function, Q is the pumping rate, r is the separation distance between the pumping and observation wells, t is time, and S is storativity. The ratio of the drawdown to the drawdown time derivative, $s'(t,r)$, can be written as (*Copty et al.*, 2011):

$$\gamma_c=\frac{s}{s'}=W(u)\exp(u) \tag{1}$$

A plot of the function γ_c is shown in Figure 1. It is observed that γ_c increases monotonically with dimensionless $1/u$ (equivalent to a dimensionless time). For a given pumping test, the ratio of the observed drawdown at any time t to its time derivative provides an estimate of u from (1). From the estimated u value, the interpreted transmissivity and storativity (T_i and S_i, respectively) corresponding to that particular moment in time are then estimated as:

$$T_i(t)=\frac{Q}{4\pi s(t)}W(u)\,;\qquad S_i(t)=\frac{4tT_i u}{r^2} \tag{2}$$

Applying the above procedure repetitively to the full duration of the test yields time-dependent estimates of the flow parameters. Thus, the CD method provides estimates of the flow parameters that change with time, in contrast to conventional methods (e.g., the Theis method) that lump all observed drawdown together to estimate single representative values of T and S.

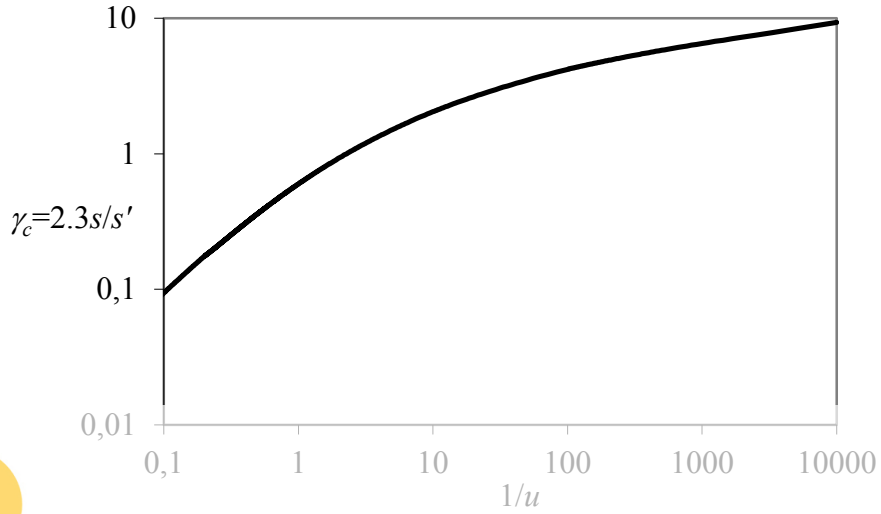


Figure 1. Plot of γ_c as a function of $1/u$ (modified from *Copty et al.*, 2011)

Through sensitivity analysis of the drawdown and its derivative to variations in the transmissivity, the interpreted transmissivity T_i-t relationship is mapped into a T_i-r^* relationship, where r^* is an radial distance computed as (*Copty et al.*, 2011):

$$r^* = \sqrt{\frac{4tT}{1.65S}}. \quad (3)$$

Equation (3) indicates that there is a direct mapping between the values of r^* and t. *Copty et al.* (2011) applied the CD method to synthetically generated 2D aquifers and found that the curves $T_i(r^*)$ match well to the function $T_g(r)$, defined as the geometric mean of the transmissivity, computed over a circular area of the aquifer centered around the pumping well and with radius r. As r increases, $T_g(r)$ approaches the geometric mean of the entire transmissivity field. Therefore, observation points located at a small distance from the pumping well (compared to the integral scale of T) would yield the most information about the spatial variability of T.

2.2. Bayesian Approach for the Estimation of the Variance and Integral Scale

Since the estimation of the transmissivity variance and integral scale is generally difficult and therefore associated with a high level of uncertainty, we define these two parameters as random functions. Denoting V and I as the variance and integral scale random functions, respectively, the primary goal of this paper is to estimate their conditional joint probability

density function (pdf), $f^c_{V,I}(v,i|Y_1 \cdots Y_N)$, where $Y_1 \cdots Y_N$ denotes the drawdown data from N available pumping tests. The superscript c denotes conditional.

Using the CD method, the drawdown data from each pumping test is converted to the geometric mean of the transmissivity as a function of radial distance from the well, $T_g(r)$. Interpretation of each pumping test is done separately. If data from more than one observation well are present for the same pumping test, they would yield similar T estimates as they would be sampling the same aquifer volume. Under such conditions, it is sufficient to use data from only one observation well. This redundancy in information has also been noted by other researchers, such as *Leven and Dietrich* (2006) and *Bohling and Butler* (2010), who demonstrated the issue of reciprocity of sequential pumping tests when pumping and monitoring wells are reversed. Limitations of reciprocity have been also explored elsewhere (e.g., *Delay et al.*, 2012; *Sanchez-Vila et al.*, 2016). Substituting each pumping test by the transmissivity functions derived from the available pumping tests, the conditional joint pdf is rewritten as $f^c_{V,I}(v,i|T_{g,1}(r) \cdots T_{g,N}(r))$, where $T_{g,1}(r) \cdots T_{g,N}(r)$ denotes the transmissivity estimates derived from pumping tests 1,…*N*. In other words, the goal here can be restated as the estimation of the joint pdf of V and I conditioned on the estimates of the geometric mean of the T field as a function of radial distance derived from all available pumping tests. To simplify the notation, the variable r is dropped from the ensuing derivations. It is however important to note that $T_{g,k}$ is not a single value but rather a full function of r.

Using Bayes' Theorem on conditional probability (e.g. *Tarantola*, 1987), the joint pdfs are:

$$f^c_{V,I}(v,i|Y_1 \cdots Y_N) = f^c_{V,I}(v,i|T_{g,1} \cdots T_{g,N}) = \frac{f_T(T_{g,1} \cdots T_{g,N}|v,i) \times f_{V,I}(v,i)}{f_T(T_{g,1} \cdots T_{g,N})} \quad (4)$$

where

$f_T(T_{g,1} \cdots T_{g,N}|v,i)$ is the likelihood of observing $T_{g,k}$ given that variance and integral scale values are v and i, respectively. This pdf can be seen as the reverse of the desired pdf, $f^c_{V,I}(v,i|T_{g,1} \cdots T_{g,N})$

$f_T(T_{g,1} \cdots T_{g,N})$ is the unconditional pdf of observing $T_{g,1} \cdots T_{g,N}$

247 $f_{V,I}(v,i)$ is the prior joint pdf of observing the variance and integral scale values
248 v and i, respectively.

249 The pdf in the denominator of (4) is denoted as ω, and can be expressed from the definitions
250 of the marginal and conditional probabilities (*Tarantola*, 1987) as:

251 $$\omega = f_T\left(T_{g,1}\cdots T_{g,N}\right) = \int_{V,I} f_T\left(T_{g,1}\cdots T_{g,N}\middle|v,i\right)\times f_{V,I}(v,i)dv\,di \qquad (5)$$

252 In words, the pdf of $T_{g,1}\cdots T_{g,N}$ is equal to the probability of observing $T_{g,1}\cdots T_{g,N}$ given that
253 V=v and I=i, integrated over all possible values of V and I; ω is a normalizing parameter that
254 guarantees that (4) is a proper pdf; that is: $\int_{V,I} f^c_{V,I}\left(v,i\middle|T_{g,1}\cdots T_{g,N}\right)dv\,di = 1$

255 If the separation distances between the different pumping tests is large such that the cones
256 of depression do not significantly overlap (consequently, there is little redundancy in the
257 data), then the pumping tests can be treated as independent (i.e., they sample different
258 volumes of the aquifer). The likelihood function $f_T\left(T_{g,1}\cdots T_{g,N}\middle|v,i\right)$ can be re-written as a
259 product of the individual pdfs:

260 $$f^c_{V,I}\left(v,i\middle|Y_1\cdots Y_N\right) = \frac{1}{\omega} f_T\left(T_{g,1}\middle|v,i\right)\ldots f_T\left(T_{g,N}\middle|v,i\right)f_{V,I}(v,i) \qquad (6)$$

261 where

262 $$\omega = \int_{V,I} f_T\left(T_{g,1}\middle|v,i\right)\ldots f_T\left(T_{g,N}\middle|v,i\right)f_{V,I}(v,i)dv\,di \qquad (7)$$

263 Equation (6) states that the pdf of V and I conditional on the available pumping test data can
264 be expressed in terms of products of N+1 pdfs. The first one, $f_{V,I}(v,i)$, is the prior joint pdf
265 of V and I, which reflects the level of knowledge of the site *prior* to conducting the pumping
266 tests. Such information can be derived from previously conducted geologic or geophysical
267 studies, or adopted from other sites with similar characteristics. In the absence of
268 information, $f_{V,I}(v,i)$, can be taken as some uniform (uninformative) distribution that
269 includes all possible values, reflecting the lack of knowledge of the site.

270 The remaining N pdfs are $f_T\left(T_{g,k}\middle|v,i\right)$ $k = 1,\cdots N$; i.e., the individual likelihood functions of
271 observing $T_{g,k}$ given that the aquifer variance and integral scale are v and i, respectively, in
272 pumping test k. As it will be described in the following subsection, the likelihood functions
273 can be readily computed without the need for any inverse modeling by generating multiple
274 realizations of the transmissivity field with different values of V and I, computing the

resultant pdf of the geometric mean of the generated transmissivity fields and then evaluating the likelihood of $T_{g,k}$. Hence, it can be seen that the desired pdf, $f^c_{V,I}\left(v,i\middle|Y_1\cdots Y_N\right)$ depends on both prior information about the site, $f_{V,I}(v,i)$, and the information derived from the pumping test, $f_T\left(T_{g,k}\middle|v,i\right)k=1,\cdots N$.

Finally, the marginal pdfs of V and I are computed as:

$$f^c_V\left(v\middle|Y_1\cdots Y_N\right)=\int_I f^c_{V,I}\left(v,i\middle|Y_1\cdots Y_N\right)di\,, \tag{8}$$

$$f^c_I\left(i\middle|Y_1\cdots Y_N\right)=\int_V f^c_{V,I}\left(v,i\middle|Y_1\cdots Y_N\right)dv\,. \tag{9}$$

The expected values of the variance and integral scale can be computed from the integral of the conditional joint pdf of V and I, $f^c_{V,I}\left(v,i\middle|Y_1\cdots Y_N\right)$:

$$E[I]=\int_{V,I} i f^c_{V,I}\left(v,i\middle|Y_1\cdots Y_N\right)dv\;di\,, \tag{10}$$

$$E[V]=\int_{V,I} v f^c_{V,I}\left(v,i\middle|Y_1\cdots Y_N\right)dv\;di\,. \tag{11}$$

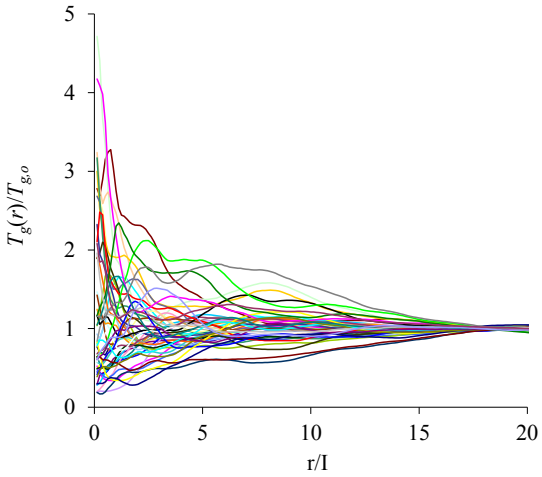
2.3. Estimation of the likelihood function $f_T\left(T_{g,1}\cdots T_{g,N}\middle|v,i\right)$

This section describes the method used to estimate the likelihood function $f_T\left(T_{g,1}\cdots T_{g,N}\middle|v,i\right)$. It is assumed that ln$T$ is a multivariate Gaussian random spatial function with exponential semi-variogram. Other semi-variogram functions could also be considered. Multiple realizations (n=1000) of the natural logarithm of the transmissivity were randomly generated for various V and I values using the Turning band method (*Mantoglou and Wilson*, 1982). The geometric mean of the transmissivity over a circular area with radius r located at the center of the generated domain was computed as:

$$T_g(r)=\exp\left[\int_{r=0}^{r}\ln(T)dA\right] \tag{12}$$

Figure 2 displays $T_g(r)$ for randomly selected transmissivity fields with variance V=1. The radial distance in the figure is normalized by the integral scale, I, while the ensemble geometric mean, $T_{g,o}=T_g(r\to\infty)$ was used to normalize the vertical axis. It can be seen

300 that the variability of $T_g(r)$ decreases as r increases. For radial distances larger than about
301 $20I$, $T_g(r)$ approached the ensemble geometric mean for all of the generated transmissivity
302 fields.
303



304
305 Figure 2. $T_g(r)$ as a function of radial distance for randomly selected transmissivity fields
306 with V=1. $T_g(r)$ is normalized by the ensemble mean of T used in data generation. The
307 distance r is normalized by the integral scale, I.
308
309 Figure 3 shows the expected value and upper/lower deciles of $T_g(r)$ for V=1, 2 and 4. The
310 expected value was computed for each distance r as the arithmetic average of the 1000
311 realizations. Similar curves for other values of the variance could be developed readily.
312 Analysis of the generated realizations shows that 1000 simulations were sufficient (with
313 error less than 1%). Figure 3 shows that for r=0 the expected value is simply the arithmetic
314 mean of the transmissivity at the well. For $r/I > 20$, $T_g(r)$ of each realization approaches the
315 ensemble geometric mean and hence, the expected value over all realizations would also
316 approach the ensemble geometric mean. The semi-variogram model selected influences the
317 rate of change with distance, but not the end points.
318 Although Figure 3 depicts only the average and upper/lower deciles, it is evident that for a
319 particular value of V and r/I, there is a range of possible values of $T_g(r)$. This range increases
320 with the increase in the variance value, and decreases as r/I increases. This figure also shows
321 overlap among the different set of curves; e.g., for a given distance, the possible range of
322 values of T_g obtained with variance V=2 is fully comprised within the range spanned by V=4.

This overlap has an influence on the Bayesian estimation, as discussed in detail is section 3.2.

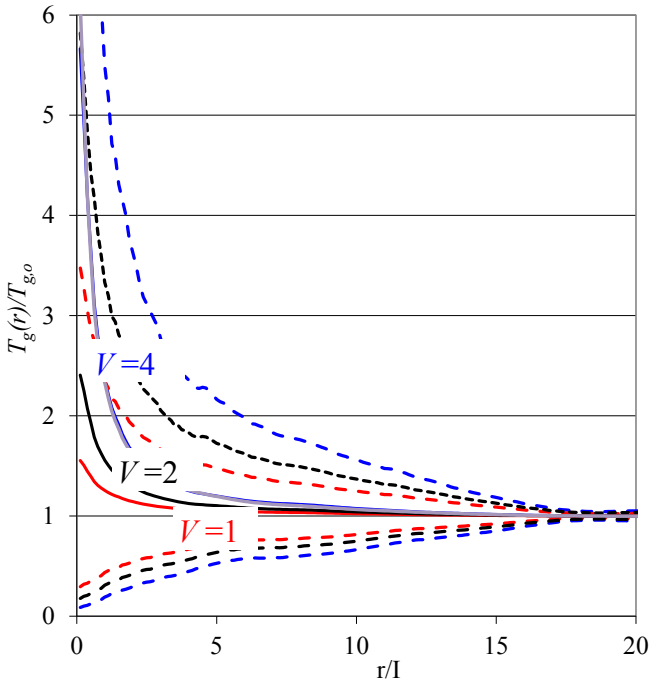


Figure 3. Expected value (solid line) and upper/lower deciles (dashed lines) for V=1, 2 and 4. The red, black and blue lines correspond to V=1, 2, and 4, respectively. $T_g(r)$ is normalized by the geometric mean of the transmissivity, T_{go} used in data generation.

Based on the information shown in Figure 3, it is possible to construct a distribution of all possible $T_g(r)$ values corresponding for each V and r/I pairs. Figure 4 shows the pdfs of $T_g(r)$ at 3 different distances: r/I=1, 5 and 10, and for V=1. As distance increases, the statistical distribution becomes narrower and less skewed. It is important to note that these pdf's are computed only once and can be used in other problems provided the semi-variogram model is kept.

Figure 4 also shows a sample calculation of the likelihood function for a $T_g(r)$ obtained from a given pumping test. Starting from the $T_g(r)$ values derived from the pumping test, one can calculate the pdf corresponding for each V and I pairs. Because the pdf's depicted in Figure 4 are for particular values of V and I, this calculation has to be repeated for all possible V and I pairs as defined by their prior joint distribution, $f_{V,I}(v,i)$.

According to the Bayesian formulation (Equation 4), the desired joint conditional pdf of V and I is function of the product of the likelihood function and the prior distribution. If for a

given pair (v,i), the product of $f_{V,I}(v,i)$, and $f_T\left(T_{g,1}\cdots T_{g,N}\middle|v,i\right)$ is small, the probability of the transmissivity field having these v and i values would also be small. On the other hand, if this product is large, this would mean that this (v, i) pair is more likely.

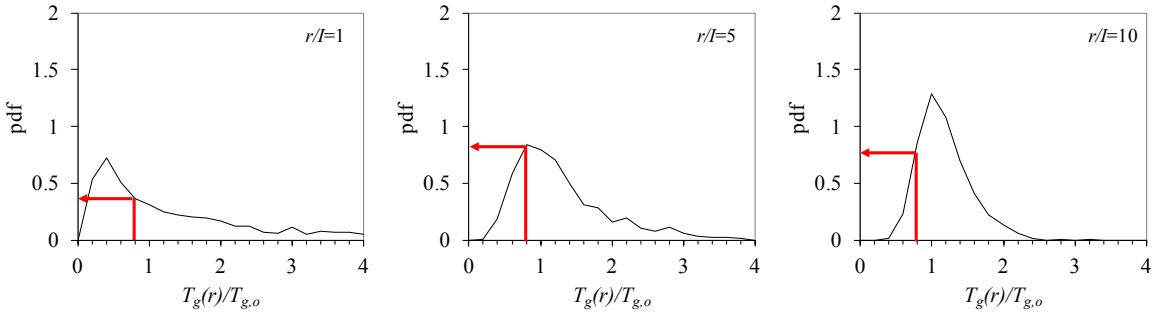


Figure 4: pdfs of $T_g(r)$ at r/I=1, 5 and 10 and for V=1. The red arrow represents the likelihood function for an example T value derived from a particular pumping test

The above discussion illustrates the benefits of formulating the parameter estimation within a Bayesian framework. First, it incorporates the information inferred from the pumping test data, as well as any prior information about the site. Second, the Bayesian formulation simplifies the calculation by expressing the desired conditional pdf, $f^c_{V,I}\left(v,i\middle|T_{g,1}\cdots T_{g,N}\right)$ in terms of its reciprocal, $f_T\left(T_{g,1}\cdots T_{g,N}\middle|v,i\right)$ (Eq. 4). Whereas the former can viewed as a form of the inverse problem and its evaluation is not straight forward, $f_T\left(T_{g,1}\cdots T_{g,N}\middle|v,i\right)$ can be readily determined from the randomly generated transmissivity fields corresponding to the v and i values as presented above without the need for any inverse modeling. Third, the Bayesian approach provides an estimate of the entire pdf based on prior information and the pumping test data and, as such, provides a measure of the uncertainty of the estimates.

In summary, we list below the main steps for the estimation of the conditional joint pdf of V and I, $f^c_{V,I}\left(v,i\middle|T_{g,1}\cdots T_{g,N}\right)$:

1. Given N pumping tests, the geometric transmissivity as a function of radial distance $T_{g,1}(r)\cdots T_{g,N}(r)$ is estimated using the CD method. Each pumping test is analyzed separately.
2. The prior joint pdf of V and I, $f_{V,I}(v,i)$, is defined based on prior information about the site.

3. For the available pumping tests, the likelihood function $f_T\left(T_{g,1}\cdots T_{g,N}\middle|v,i\right)$ is determined from Figures 3 and 4. By assuming the pumping tests are sufficiently far and, therefore, can be treated as independent, the likelihood function is expressed as a product of the likelihood functions of the individual pumping tests (Eq. 6). It is important to note that these figures do not require the simulation of the groundwater flow equation; they were developed by generated multiple realizations of the transmissivity field and averaging the T as a function of radial distance. The calculation of the likelihood function is repeated for all possible v and i pairs as defined by their prior distribution (step 2).
4. The normalizing parameter, ω, is calculated from Eq. (5) or Eq. (7) if the pumping tests treated as independent.
5. The desired conditional pdf is finally computed according to Eq. (4) or Eq. (6). The marginal distributions of V and I are determined from Eq (8) and Eq. (9), respectively.

3. Application

3.1. Data Generation

To demonstrate the above parameter estimation procedure, the procedure was tested using 1000 synthetic pumping tests conducted in confined heterogeneous aquifers. The heterogeneous transmissivity fields were generated using the turning bands method. It was assumed that the natural log transform of the transmissivity is a multivariate Gaussian random spatial function with zero mean (T_g=1), an exponential semi-variogram, with variance, V=1, and integral scale, I= 8 length units (lu). Storativity was assumed to be uniform, as field data usually indicate that the spatial variation in storativity is less than that of the transmissivity. The storativity value used in all simulations was 0.0001; which is a typical value for a confined aquifers (*Domenico and Schwartz*, 1997).

The flow domain was assumed to be 481 by 481 lu. A fully penetrating pumping well was placed at the center of the domain. The observation point was assumed to be at a distance of I/8 from the pumping well. Constant head conditions were prescribed along the outer boundaries of the domain. The duration of the pumping test was τ=1, while the pumping rate was fixed at Q=2 (using consistent units for both τ and Q). Pumping tests were terminated before the drawdown data were affected by boundary effects.

398 The pumping tests were simulated using MODFLOW (*Harbaugh et al*., 2000). A uniform
399 grid of 1 by 1 lu was used. The drawdown data were analyzed using the CD method yielding
400 one $T_g(r)$ for each of the 1000 simulated pumping tests. Using the proposed Bayesian
401 approach, the inferred $T_g(r)$ was then used to estimate the variance and integral scale. To
402 assess the robustness of the proposed method, a Monte Carlo approach was adopted. First,
403 each of the $T_g(r)$ curves were used independently to estimate the variance and integral scale
404 of the T field. This corresponds to the case when only a single pumping test is present (N=1).
405 The method was then repeated by combining 5 and 10 pumping tests (N =5 and N =10,
406 respectively) to test the performance of the method when multiple wells are present.
407 The Bayesian estimation requires the definition of a prior distribution for the parameters of
408 interest (variance and integral scale). In the present analysis, the prior distribution of the
409 variance was assumed to be uniform between 0 and 5, $U_V(0,5)$. This range encompasses
410 typical variance values encountered in the field (Gelhar, 1993). The prior pdf of the integral
411 scale was also assumed to be uniform between 0 and 40 lu, $U_I(0,40)$. The uniform
412 distributions are the least informative distributions in terms of priors, requiring only the
413 definition of upper limits (5 and 40 lu, respectively). The corresponding joint prior pdf is
414 $f_{V,I}(v,i)=1/5\times1/40=0.005$. The joint pdf is also uniformly distributed which means that all v
415 and i pairs falling between the lower and upper limits of V and I respectively have the same
416 probability of occurring. To assess the sensitivity of the prior distribution on the estimation
417 of the variance and integral scale, the analysis was also repeated assuming the prior
418 distributions of the variance and the integral scale are $U_V(0,3)$ and $U_I(0,30)$, respectively,
419 which are closer to the parameter values used in data generation.
420
421 **3.2. Results**
422 The parameter estimation procedure was repetitively applied to all 1000 pumping tests.
423 Figure 5 shows a randomly selected example of the conditional joint pdf of the variance and
424 integral scale obtained with the Bayesian estimation procedure. The true variance and
425 integral scale used in the data generation are 1 and 8 lu, respectively. The number of available
426 pumping tests was 5. The conditional pdf joint should be contrasted to the prior
427 $f_{V,I}(v,i)=0.005$. This figure shows that conditioning on the pumping test data shifts the pdf
428 from the diffuse prior towards the true values of the variance and integral scale (v=1, i=8 lu).
429 The range of the more likely values of the variance and integral scale significantly decreased.
430

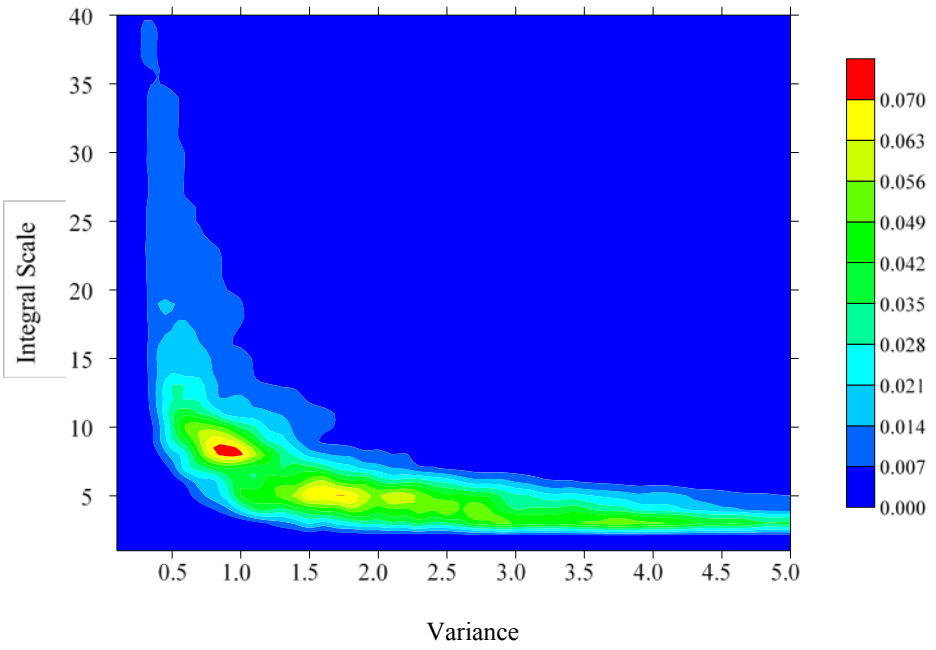


Figure 5. Example of the conditional joint pdf of the variance and integral scale based on data from 5 pumping tests. The prior distributions of the variance and integral scale are $U_V(0,5)$ and $U_I(0,40)$ which correspond to a prior pdf $f_{V,I}(v,i)=0.005$. The true values are $V=1$ and $I=8$ lu.

The marginal distributions of the integral scale and variance for 3 randomly selected cases are shown in Figure 6. Each of these conditional pdfs were computed assuming 5 pumping tests were available. The mean of the marginal pdfs of the integral scale for the three randomly selected cases were 5.8, 9.2 and 17 lu. The mean of the marginal pdfs of the variance on the other hand were 2.4, 1.8 and 0.86. For comparison, the prior pdfs of V and I are also shown in this figure. The corresponding means of the prior pdfs of the integral scale and variance were 20 lu and 2.5, respectively. These results show that the conditional variance and integral scale marginal pdfs are closer to the true values ($V=1$, $I=8$ lu) compared to the initial prior distribution. The conditional marginal pdfs do exhibit a tail that results from the diffuse prior distribution of V and I, and the overlap of the likelihood functions (Figures 3 and 4).

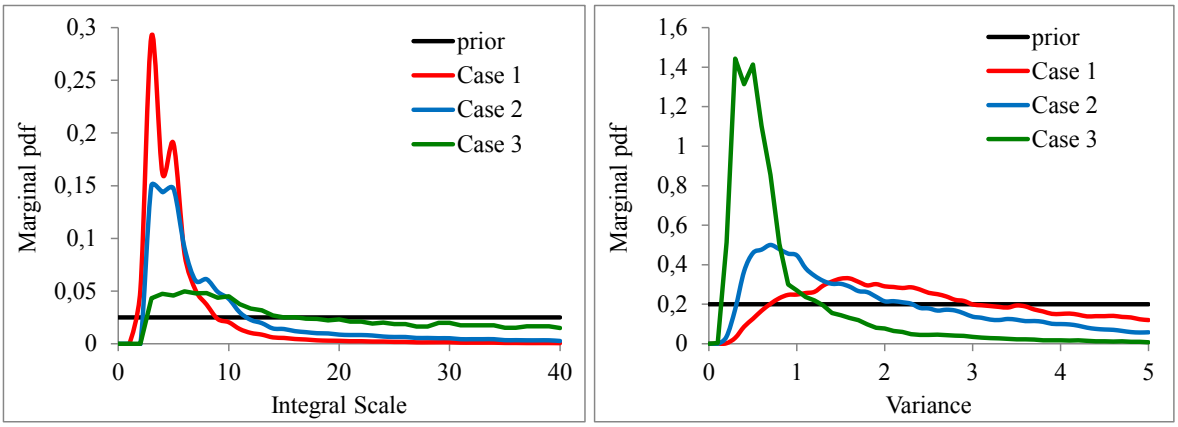
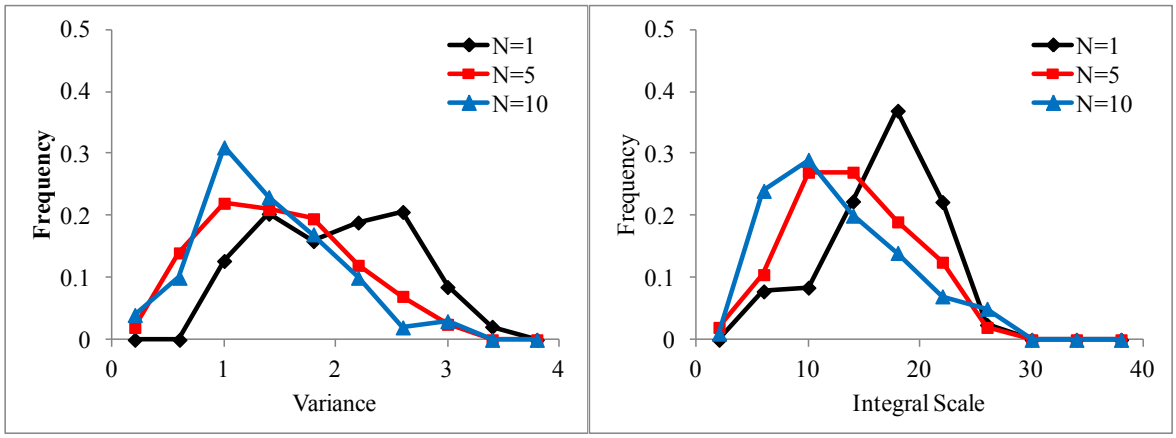


Figure 6. Integral scale and variance marginal pdfs for three randomly selected cases. Each of these cases assumes 5 pumping tests are available. The prior distributions of the variance and integral scale are $U_V(0,5)$ and $U_I(0,40)$. The true values are V=1 and I=8 lu.

Figure 7 presents the histogram of the conditional expected values of the integral scale (E[I]) and variance (E[V]), from the 1000 Monte Carlo results. The results are computed using 1, 5 or 10 pumping tests. The average of E[V] and E[I] over all realization for N=1, 5, and 10 are shown in Table 1, For comparison, the "true" values of V and I used in the generation of the T fields and the expected values of the prior distribution are also included. Figure 7 and Table 1 demonstrate that the Bayesian updating can be viewed as a weighted average of the prior pdf and the results of the pumping test. Conditioning improves the estimation of the considered variables although, because of the overlap of the different likelihood functions (Figures 3), the resulting histograms still show some spread. Provided there is no redundancy in the data, increasing the number of pumping tests causes the estimates of the variance and integral scale to shift towards the true values.



467 Figure 7. Histograms of E[V] and E[I] based on the Monte Carlo analysis, assuming 1, 5 or
468 10 pumping tests are available. The prior distributions are $U_V(0,5)$ and $U_I(0,40)$, implying
469 expected values of 2.5 and 20 lu, respectively. The true values are V=1 and I=8 lu.
470
471 Table 1: Average of E[V] and E[I] for all simulations, assuming N=1, 5 or 10 pumping tests
472 are available and for different prior distributions of the variance and integral scale. For
473 comparison, the true values used in the generation of the transmissivity field are also shown

Prior distributions	Number of Pumping Tests	Average of E[V]	Average of E[I], lu
V: Uniform between 0 and 5 *I*: Uniform between 0 and 40 lu	0	2.5	20
	1	1.96	16.7
	5	1.47	13.9
	10	1.36	12.4
V: Uniform between 0 and 3 *I*: Uniform between 0 and 30 lu	0	1.5	15
	1	1.36	13.8
	5	1.21	12.5
	10	1.17	11.5
"True" Values of *I* and *V*		1	8

474 Note: The average values corresponding to N=0 are the values of the prior distributions
475 before conditioning on the pumping well data
476
477 To assess the impact of the prior V and I distributions, the parameter estimation procedure
478 was repeated with the same pumping tests, but now assuming that the initial distributions of
479 the variance and integral scales are uniformly distributed between 0 and 3 and between 0
480 and 30 lu, respectively. Figure 8 shows the histograms of the E[V] and E[I] for different
481 number of pumping tests. The corresponding average of E[V] and E[I] for all simulations are
482 given in Table 1. With increase in the number of pumping tests, E[V] and E[I] move from
483 the expected values of the prior distributions, $E^p[V]$ =1.5 and $E^p[I]$=15 lu, towards the true
484 parameter values, V=1 and I=8 lu. Compared to Figure 7, the impact of the number of tests
485 on the estimation is less significant (in particular for E[V]), because the prior estimates were

closer to the true values. This demonstrates the benefits of using accurate prior distributions in Bayesian estimation procedures provided such information is available.

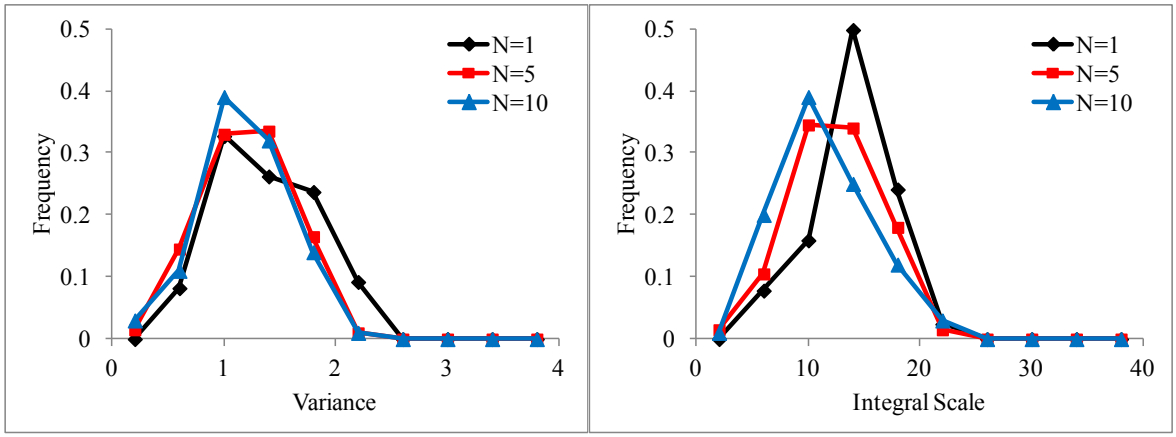


Figure 8. Histograms of E[V] and E[I], assuming 1, 5 or 10 pumping tests are available. The prior distributions are $U_V(0,3)$ and $U_I(0,30)$, implying expected values of 1.5 and 15 lu, respectively. The true values are V=1 and I=8 lu.

4. Summary and Conclusions

Modeling of the spatial variability of transmissivity is essential for the accurate simulation of groundwater flow and contaminant transport. The spatial variability of T is commonly defined in terms of a semi-variogram or covariance function that is expressed in terms of two statistical parameters: the variance, V, and integral scale, I. It is therefore important to develop simple techniques for the estimation of these two statistical parameters. Despite the development in recent years of novel data acquisition techniques, the analysis of drawdown data from pumping tests remain the most commonly used technique for the identification of subsurface flow parameters. Traditionally, the interpretation of pumping tests generally yield single representative (apparent) estimates of the flow parameters. Here we explore whether pumping test data can be used to infer the variance and integral scale of the transmissivity, two statistical parameters that describe the spatial variability of the underlying transmissivity field. Estimates of the variance and integral scale can be employed in the analysis of flow and contaminant transport problems and their associated uncertainty, either directly using various analytical expressions found in the literature that relate flow and transport attributes

to the underlying aquifer heterogeneity, or numerically through the generation of multiple realizations of the transmissivity field.

The starting point of the present study is the Continuous Derivation method (*Copty et al.*, 2011), which uses the drawdown and its time derivative to estimate a function that was shown to be close to the geometric mean of the transmissivity field defined over an increasing radial distance from the pumping well, $T_g(r)$. Analysis of $T_g(r)$ indicated that the early part of the curve is sensitive to the variance of the T field while the rate at which it approaches the geometric mean of T in the full domain could be related to the integral scale. This provided the basis for attempting to use $T_g(r)$ for estimating V and I.

The estimation of V and I was formulated using a Bayesian approach which expresses the conditional pdf of V and I as a weighted function of the prior pdf and the likelihood function that is itself dependent on the pumping test data. An important advantage of this approach is that the likelihood function is readily computed from multiple realizations of the transmissivity without the need to solve potentially complex inverse problems. Another feature of the Bayesian approach is that it provides a measure of the uncertainty of the estimated statistical parameters.

The Bayesian estimation procedure was applied to a number of synthetic pumping tests. The analysis assumed that the natural log transform of the transmissivity distribution is a multivariate Gaussian random spatial function with an exponential variogram. The variance and integral scale were assumed to have a uniform joint prior distribution. The diffuse prior distributions considered in this application and the non-uniqueness of the likelihood function means that the results of the estimation procedure can be associated with a significant level of uncertainty, highlighting the challenges of the parameter estimation problem. Single as well as multiple pumping tests (N=5 and N=10) were assumed to be available. In the case when multiple pumping tests were available, it was further assumed that they are located far from each other such they sample different portions of the aquifer.

The significance of the Bayesian estimation procedure becomes apparent when the conditional distribution of V and I is compared to the prior pdf of V and I which represents the level of information available prior to conducting the pumping tests. It is shown that improved estimates of V and I are obtained as the number of available pumping tests increases or when more accurate prior distributions are available. The results of this numerical example show that as little as 5 pumping tests may be sufficient to yield reliable estimates of the statistical parameters of the transmissivity field.

Overall, the proposed interpretation procedure can be viewed as an extension of traditional pumping test interpretation procedures, such as the Theis method, that besides best-fit estimates of the storativity and transmissivity, can potentially also provide estimates of the variance and integral scale of the transmissivity field.

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